

# On the distribution of entanglement changes produced by unitary operations

J. Batle<sup>1</sup>, A. R. Plastino<sup>1,2,3</sup>, M. Casas<sup>1</sup>, and A. Plastino<sup>3,4</sup>

<sup>1</sup>*Departament de Física, Universitat de les Illes Balears, 07071 Palma de Mallorca, Spain*

<sup>2</sup>*Faculty of Astronomy and Geophysics, National University La Plata, C.C. 727, 1900 La Plata*

<sup>3</sup>*Argentina's National Research Council (CONICET)*

<sup>4</sup>*Department of Physics, National University La Plata, C.C. 727, 1900 La Plata, Argentina*

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## Abstract

We consider the change of entanglement of formation  $\Delta E$  produced by a unitary transformation acting on a general (pure or mixed) state  $\rho$  describing a system of two qubits. We study numerically the probabilities of obtaining different values of  $\Delta E$ , assuming that the initial state is randomly distributed in the space of all states according to the product measure recently introduced by Zyczkowski *et al.* [Phys. Rev. A **58** (1998) 883].

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Theory

Entanglement is one of the most fundamental issues of quantum theory [1]. It is a physical resource, like energy, associated with the peculiar non-classical correlations that are possible between separated quantum systems. Recourse to entanglement is required so as to implement quantum information processes [2–9] such as quantum cryptographic key distribution [10], quantum teleportation [11], superdense coding [12], and quantum computation [13–15]. Indeed, production of entanglement is a kind of elementary prerequisite for any quantum computation. Such a basic task is accomplished by unitary transformations  $\hat{U}$  (quantum gates) representing quantum evolution acting on the space state of multipartite systems.  $\hat{U}$  should describe nontrivial interactions among the degrees of freedom of its subsystems. How to construct an adequate set of quantum gates is one of the fundamental questions about quantum computation. A pleasing answer is found. Any generic two-qubits gate suffices for universal computation [16]. One would then be interested in ascertaining just how efficient distinct  $\hat{U}$ 's are as entanglers. Quite interesting work has recently been performed to this effect (see, for instance, [17–21]).

A state of a composite quantum system is called “entangled” if it can not be represented as a mixture of factorizable pure states. Otherwise, the state is called separable. The above definition is physically meaningful because entangled states (unlike separable states) cannot be prepared locally by acting on each subsystem individually [22,23].

A physically motivated measure of entanglement is provided by the entanglement of formation  $E[\rho]$  [24]. This measure quantifies the resources needed to create a given entangled state  $\rho$ . That is,  $E[\rho]$  is equal to the asymptotic limit (for large  $n$ ) of the quotient  $m/n$ , where  $m$  is the number of singlet states needed to create  $n$  copies of the state  $\rho$  when the optimum procedure based on local operations is employed. The entanglement of formation for two-qubits systems is given by Wootters’ expression [25],

$$E[\rho] = h\left(\frac{1 + \sqrt{1 - C^2}}{2}\right), \quad (1)$$

where

$$h(x) = -x \log_2 x - (1 - x) \log_2 (1 - x), \quad (2)$$

and  $C$  stands for the *concurrence* of the two-qubits state  $\rho$ . The concurrence is given by

$$C = \max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4), \quad (3)$$

$\lambda_i$ , ( $i = 1, \dots, 4$ ) being the square roots, in decreasing order, of the eigenvalues of the matrix  $\rho\tilde{\rho}$ , with

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y) \rho^* (\sigma_y \otimes \sigma_y). \quad (4)$$

The above expression has to be evaluated by recourse to the matrix elements of  $\rho$  computed with respect to the product basis.

In the present effort we will concern ourselves with one of the basic constituents of any quantum processing device: *quantum logic gates*, i.e., unitary evolution operators  $\hat{U}$  that act on the states of a certain number of qubits. If the number of such qubits is  $m$ , the quantum gate is represented by a  $2^m \times 2^m$  matrix in the unitary group  $U(2^m)$ . These gates are reversible: one can reverse the action, thereby recovering an initial quantum state from a final one. We shall work here with  $m = 2$ . The simplest nontrivial 2-qubits operation is the quantum controlled-NOT, or CNOT (equivalently, the exclusive OR, or XOR). Its classical counterpart is a reversible logic gate operating on two bits:  $e_1$ , the control bit, and  $e_2$ , the target bit. If  $e_1 = 1$ , the value of  $e_2$  is negated. Otherwise, it is left untouched. The quantum CNOT gate  $C_{12}$  (the first subscript denotes the control bit, the second the target one) plays a paramount role in both experimental and theoretical efforts that revolve around the quantum computer concept. In a given orthonormal basis  $\{|0\rangle, |1\rangle\}$ , and if we denote addition modulo 2 by the symbol  $\oplus$ , we have [26]

$$|e_1\rangle |e_2\rangle \rightarrow C_{12} \rightarrow |e_1\rangle |e_1 \oplus e_2\rangle. \quad (5)$$

In conjunction with simple single-qubit operations, the CNOT gate constitutes a set of gates out of which *any quantum gate may be built* [16]. In other words, single qubit and CNOT gates are universal for quantum computation [16].

As stated, the CNOT gate operates on quantum states of two qubits and is represented by a 4x4-matrix. This matrix has a diagonal block form. The upper diagonal block is just

the identity 2x2 matrix. The lower diagonal 2x2 block is the representation of the one-qubit NOT gate  $U_{NOT}$ , of the form

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (6)$$

A related operator is  $\hat{U}_\theta$ , for which the lower diagonal block is of the form

$$\begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \quad (7)$$

$C_{12}$  is able to transform factorizable pure states into entangled ones, i.e.,

$$C_{12} : [c_1|0\rangle + c_2|1\rangle]|0\rangle \leftrightarrow c_1|0\rangle|0\rangle + c_2|1\rangle|1\rangle, \quad (8)$$

and this transformation can be reversed by applying the same CNOT operation once more [26]. In general, the action of  $\hat{U}_{CNOT}$  ( $\hat{U}_\theta$ ) on a 2-qubits state (pure or mixed) produces a change of entanglement  $\Delta E$ .

The two-qubits systems with which we are going to be concerned here are the simplest quantum mechanical systems exhibiting the entanglement phenomenon and play a fundamental role in quantum information theory. The concomitant space  $\mathcal{H}$  of *mixed states* is 15-dimensional and its properties are not of a trivial character. There are still features of this space, related to the phenomenon of entanglement that have not yet been characterized in full detail. One such characterization problem will be the center of our attention here. We shall perform a systematic numerical survey of the action of  $\hat{U}_{CNOT}$  ( $\hat{U}_\theta$ ) on our 15-dimensional space in order to ascertain the manner in which  $P(\Delta E)$  is distributed in  $\mathcal{H}$ , with  $P$  the probability of generating a change  $\Delta E$  associated to the action of these operators. This kind of exploratory work is in line with recent efforts towards the systematic exploration of the space of arbitrary (pure or mixed) states of composite quantum systems [27–29] in order to determine the typical features exhibited by these states with regards to the phenomenon of quantum entanglement [27–33]. It is important to stress the fact that we

are exploring a space in which the majority of states are *mixed*. The exciting investigations reported in [17–21] address mainly pure states.

As an illustration of the type of search we intend to perform, consider the real pure state

$$\rho = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle, (a, b, c, d \in \mathcal{R}^+), \quad a^2 + b^2 + c^2 + d^2 = 1, \quad (9)$$

whose concurrence squared is

$$C_\rho^2 = 4(ad - bc)^2, \quad (10)$$

and the transformations

$$\begin{aligned} \hat{\rho}' &= \hat{U}_{CNOT} \hat{\rho} \hat{U}_{CNOT}^{-1} \\ \hat{\rho}' &= \hat{U}_{\pi/2} \hat{\rho} \hat{U}_{\pi/2}^{-1} \\ \hat{\rho}' &= \hat{U}_{\pi/4} \hat{\rho} \hat{U}_{\pi/4}^{-1}. \end{aligned} \quad (11)$$

The ensuing squared concurrences for  $\rho'$  are, respectively,

$$\begin{aligned} C_{CNOT}^2 &= 4(ac - bd)^2 \\ C_{\pi/2}^2 &= 4(ac + bd)^2 \\ C_{\pi/4}^2 &= 2(a^2 + b^2)(c^2 + d^2) + 4[(-a^2 + b^2)cd + (c^2 - d^2)ab]. \end{aligned} \quad (12)$$

Different changes of entanglement are seen to take place. The question is: given an initial degree of entanglement of formation  $E$ , what is the probability  $P(\Delta E)$  of encountering a change in entanglement  $\Delta E$  upon the action of  $\hat{U}_{CNOT}$  ( $\hat{U}_\theta$ )?

Due to the relevance of the  $\hat{U}_{CNOT}$  gate, we are going to focus our present considerations upon the probability distribution  $P(\Delta E)$  associated with  $\hat{U}_{CNOT}$ . However, we must bear in mind that the  $P(\Delta E)$ 's associated with other gates may be different from the  $P(\Delta E)$  generated by the  $\hat{U}_{CNOT}$  gate. As an illustration of this differences we also studied some features of the  $P(\Delta E)$ 's corresponding to members of the mono-parametric family of gates  $\hat{U}_\theta$ . This family of unitary operations comprises as a particular member the identity operation on two-qubits,  $I = \hat{U}_{\theta=0}$ , for which we trivially have  $P(\Delta E) = 0$  for all  $\Delta E \neq 0$ .

To answer the type of questions mentioned above we will perform a Monte Carlo exploration of  $\mathcal{H}$ . To do this we need to define a proper measure on  $\mathcal{H}$ . The space of all (pure and mixed) states  $\rho$  of a quantum system described by an  $N$ -dimensional Hilbert space can be regarded as a product space  $\mathcal{S} = \mathcal{P} \times \Delta$  [27,28]. Here  $\mathcal{P}$  stands for the family of all complete sets of orthonormal projectors  $\{\hat{P}_i\}_{i=1}^N$ ,  $\sum_i \hat{P}_i = I$  ( $I$  being the identity matrix).  $\Delta$  is the set of all real  $N$ -tuples  $\{\lambda_1, \dots, \lambda_N\}$ , with  $0 \leq \lambda_i \leq 1$ , and  $\sum_i \lambda_i = 1$ . The general state in  $\mathcal{S}$  is of the form  $\rho = \sum_i \lambda_i P_i$ . The Haar measure on the group of unitary matrices  $U(N)$  induces a unique, uniform measure  $\nu$  on the set  $\mathcal{P}$  [27,28,34]. On the other hand, since the simplex  $\Delta$  is a subset of a  $(N-1)$ -dimensional hyperplane of  $\mathcal{R}^N$ , the standard normalized Lebesgue measure  $\mathcal{L}_{N-1}$  on  $\mathcal{R}^{N-1}$  provides a natural measure for  $\Delta$ . The aforementioned measures on  $\mathcal{P}$  and  $\Delta$  lead to a natural measure  $\mu$  on the set  $\mathcal{S}$  of quantum states [27,28],

$$\mu = \nu \times \mathcal{L}_{N-1}. \quad (13)$$

We are going to consider the set of states of a two-qubits system. Consequently, our system will have  $N = 4$  and, for such an  $N$ ,  $\mathcal{S} \equiv \mathcal{H}$ . All our present considerations are based on the assumption that the uniform distribution of states of a two-qubit system is the one determined by the measure (13). Thus, in our numerical computations we are going to randomly generate states of a two-qubits system according to the measure (13) and study the entanglement evolution of these states upon the action of quantum logical gates  $U_\theta$ .

Before embarking in our exploration of the entanglement changes produced by unitary operations, it is convenient to briefly review the salient features of the distribution of entanglement on the state-space  $\mathcal{H}$  of two-qubits. Fig. 1a plots the probability  $P(E)$  of finding two-qubits states of  $\mathcal{H}$  endowed with a given amount of entanglement of formation  $E$ . The solid line corresponds to all states (pure and mixed), while the dashed curve depicts pure state behavior only. We clearly see that our probabilities are of a quite different character when they refer to pure states than when they correspond to mixed ones. Most mixed states have null entanglement, or a rather small amount of it, while the entanglement of pure states is more uniformly distributed. (see the enlightening discussion in [27]).

Fig. 1b plots the probability  $P(E_F)$  of generating via the CNOT gate a final state (pure or mixed) with entanglement  $E_F$  if the initial entanglement is zero (solid line). The mean amount of CNOT-generated entanglement from an initial state with  $E = 0$  is  $\langle E_F \rangle = 0.0052$ . For the  $\pi/4$ -gate this figure equals 0.0023. For the sake of comparison we plot alongside the solid line a dashed curve that depicts the probability  $P(E)$  of randomly selecting a state endowed with an entanglement  $E$ . We encounter a mean entanglement  $\langle E \rangle = 0.03$ . We appreciate the fact that it is quite unlikely that we may generate, via the CNOT gate, a significant amount of entanglement if the initial state is separable.

Our gates act on an initial state of entanglement  $E_0$  and produces a final state of entanglement  $E_F$ . In Fig. 2 we study (for all states) how the mean final entanglement  $\langle E_F \rangle$  depends on the initial entanglement  $E_0$ . The final states are generated via i) the CNOT (solid line), ii) the  $\hat{U}(\theta = \pi/3)$  (dot-dashed line), iii) the  $\hat{U}(\theta = \pi/4)$  (dashed line), iv) the  $\hat{U}(\theta = \pi/6)$  (dotted line), and v) the  $\hat{U}(\theta = 0)$  (thin dashed line) gates. On average, these gates tend to disentangle the initial state. Here we have, of course, the trivial exception of the identity gate,  $\theta = 0$ , which does not produce any change of entanglement at all. As can be expected, the “disentangling” behaviour of the  $\hat{U}(\theta)$  gate (when acting on mixed states) becomes less and less important as  $\theta$  approaches zero. As shown in the inset, the situation is different for pure states. In this case the CNOT gate (solid line) increases the mean entanglement up to  $\simeq 0.5$  for states with  $E_0$  lying in the interval  $[0, 0.5]$  and  $\langle E_F \rangle$  becomes moderately smaller than  $E_0$  for states with large entanglement. The result is similar using the  $\pi/4$  gate (dashed line) but, for small initial entanglement,  $\langle E_F \rangle$  monotonically increases with  $E_0$ , reaching the value 0.738 for  $E_0 = 1$ . The crossing between CNOT and  $\pi/4$  results takes place at  $E_0 = 0.53$ . The mean entanglement  $\langle E \rangle = \frac{1}{3 \ln 2}$  [29] for pure states is also drawn (thin “horizontal” line).

Fig. 3a is a  $P(\Delta E)$  vs.  $\Delta E$  plot *for pure states*. The CNOT gate is compared with the unitary transformation (7) with  $\theta = \pi/4$ . In both cases there is a nitid peak at  $\Delta E = 0$ . Thus, if the initial state has entanglement  $E$ , our survey indicates that the most probable circumstance is that the gate will leave it unchanged. One appreciates the fact that  $P(\Delta E)$

decreases steadily as  $\Delta E$  grows. In the case of the  $\pi/4$  gate the whole of the horizontal  $[-1, 1]$ -interval is not accessible.

It is important to bear in mind that, due to the invariance of the product measure under unitary transformations, if the initial states are uniformly distributed according to that measure, the probability distribution  $P(E_F)$  associated with the entanglement of the final states is the same as the distribution  $P(E_0)$  characterizing the entanglement of the initial states. Consequently, it is instructive to compare the distribution  $P(\Delta E)$  associated with a unitary gate with the distribution  $P_R(\Delta E)$  obtained generating the final state randomly and independently from the initial one (that is, instead of using a unitary gate to generate the final state we generate it in random fashion). The dotted-dashed curve in Fig. 3a depicts the probability  $P_R(\Delta E)$  of obtaining a difference  $\Delta E$  between the amounts of entanglement of two randomly selected pure states. This last curve serves as a reference pattern for appreciating the net gate effect, i.e., the difference between the unitary gate-governed evolution and that of a random change-of-state process. This global picture changes dramatically if we consider mixed states as well (see Fig. 3b). For both gates considered here, there is still a peak at  $\Delta E = 0$ , but of a much sharper nature.

We are going to consider next the set of initial states that, as a result of our gate operation, suffer a given, fixed entanglement's change  $\Delta E$ . To that effect we depict in Figs. 4a and 4b the behaviour of the mean initial entanglement  $\langle E_0 \rangle$  as a function of the entanglement's increase  $\Delta E$ . In other words, for each possible value of  $\Delta E$ , we calculate the mean value of the entanglement of formation associated with all those initial states yielding the (same) change of entanglement  $\Delta E$  upon the action of the CNOT or the  $\pi/4$  gates. Fig. 4a corresponds to pure states and Fig. 4b to all states. In Figs. 4c (pure states) and 4d (all states) we plot  $\langle E_0^2 \rangle - \langle E_0 \rangle^2$  vs.  $\Delta E$ . Pure states behave again in a drastically different manner as that of mixed states. We appreciate in Fig. 4a the fact that, for pure states, the CNOT exhibits the same qualitative behaviour as the  $\pi/4$  unitary transformation. The interval  $[-1, 1]$  of  $\Delta E$  for the  $\pi/4$  transformation is not wholly accessible. We see that if the average amount of entanglement is large, then the two types of action we are considering here



will tend to disentangle the initial state. If mixed states enter the scene a totally different picture emerges. At the origin ( $\Delta E = 0$ ), an appreciable *change of curvature is noticed*. Confirming the results of Fig. 3b, we see that if the initial entanglement is zero, it tends to remain so. The dispersion is largest at the origin, for pure states (Fig. 4c). Including all states (Fig. 4d) introduces once again dramatic effects, the dispersion is negligible at the origin, grows rapidly in symmetric fashion, attains symmetric maxima and then decreases steadily towards zero for large  $\Delta E$ -values. The dispersion is much larger for two states connected through the  $\pi/4$  operation than for two states connected via CNOT.

Fig. 5 depicts for the CNOT gate (left) and for the  $\pi/4$ -gate (right) the probability distribution  $P(E_F)$  vs.  $E_F$  for fixed initial entanglement  $E_0 = 0.1, 0.2, 0.3$ , and  $0.4$ , respectively. Notice that several crossings take place. No monotonous behavior can be therefore be associated to the  $E_0$ -change.

There are several information measures that are in common use for the investigation of quantum entanglement. The von Neumann measure

$$S_1 = -Tr(\hat{\rho} \ln \hat{\rho}), \quad (14)$$

is important because of its relationship with the thermodynamic entropy. On the other hand, the so called participation ratio,

$$R(\hat{\rho}) = \frac{1}{Tr(\hat{\rho}^2)}, \quad (15)$$

is particularly convenient for calculations and can be regarded as a measure of the degree of mixture of a given density matrix [17,27,30]. It varies from unity for pure states to  $N$  for totally mixed states (if  $\hat{\rho}$  is represented by an  $N \times N$  matrix). It may be interpreted as the effective number of pure states that enter the mixture. If the participation ratio of  $\hat{\rho}$  is high enough, then its partially transposed density matrix is positive, which for  $N = 4$  amounts to separability [35,36].

The so-called  $q$ -entropies, which are functions of the quantity

$$\omega_q = Tr(\hat{\rho}^q), \quad (16)$$

provide one with a whole family of entropic measures. In the limit  $q \rightarrow 1$  these measures incorporate (14) as a particular instance. On the other hand, when  $q = 2$  they are simply related to the participation ratio (15).

We revisit next how i) the mean initial entanglement  $\langle E_0 \rangle$ , and ii) the associated dispersion  $\langle E_0^2 \rangle - \langle E_0 \rangle^2$ , characterizing those initial states yielding a given increase in entanglement, behave as a function of the aforementioned entanglement's change  $\Delta E$ . We consider the action of the CNOT gate upon states having a *given amount of "mixedness"* (as measured by the participation ratio). We shall consider two such values, namely,  $R = 1.4$  (left side of Fig. 6) and  $R = 2.2$  (right side of Fig. 6). As it is expected, the maximum value of the mean initial entanglement  $\langle E_0 \rangle$  decreases as the degree of mixture ( $R$ ) increases. The corresponding graphs are depicted in Figs. 6a and 6b, which are to be compared to those of Figs. 4b and 4d, respectively. Quite significant differences are observed, specially in the case of dispersion, where we have now maxima instead of minima at the origin  $\Delta E = 0$ .

Two-qubits systems are the simplest quantum mechanical systems exhibiting the entanglement phenomenon and play thereby a fundamental role in quantum information theory. The properties of its associated, 15-dimensional space  $\mathcal{H}$  of *mixed states* are of a highly non-trivial character. As a consequence, the entanglement-related features of  $\mathcal{H}$  are the subject of continuous interest as they have not been characterized in full detail yet. In this work we have investigated one of these characterization problems: the workings of logic gates, and in particular of the controlled-NOT gate, an operation that establishes or removes entanglement of formation  $E$ .

To such an effect we performed a systematic numerical survey of the action of  $\hat{U}_{CNOT}$  (and of more general gates  $\hat{U}_\theta$ ) on our 15-dimensional space. The underlying goal was that of ascertaining the manner in which the probability  $P(\Delta E)$  of generating a change of entanglement  $\Delta E$ , associated to the action of these gates, *is distributed in  $\mathcal{H}$* .

We have found that the statistical characteristics of our gates are quite different when they operate on mixed states vis-à-vis their effect on pure states.  $\mathcal{H}$  is heavily populated with separable mixed states. We have shown that the probability of entangling these states

with our logic gates is rather low. Also, acting on an entangle mixed state is more likely that the gates will diminish the entanglement rather than augmenting it.

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## FIGURE CAPTIONS

Fig. 1-a) Probability of finding two-qubits states with a given amount of entanglement of formation  $E$ . The solid line corresponds to all states (pure and mixed) and the dotted line to pure states. b) Probability of generating via the CNOT gate a final state with entanglement  $E_F$  if the entanglement  $E_0$  of the initial state is zero (solid line). The dashed line is the probability  $P(E)$  of randomly selecting a state with entanglement  $E$ .

Fig. 2- Mean final entanglement  $\langle E_F \rangle$  vs. its initial value  $E_0$  for all states obtained via the CNOT gate (solid line), the  $\hat{U}(\theta = \pi/3)$  (dot-dashed line), the  $\hat{U}(\theta = \pi/4)$  (dashed line), the  $\hat{U}(\theta = \pi/6)$  (dotted line), and the  $\hat{U}(\theta = 0)$  (thin dashed line) gates. The inset illustrates the concomitant results for pure states.

Fig. 3- a)  $P(\Delta E)$  vs.  $\Delta E$  for pure states. The change of entanglement  $\Delta E$  arises as a result of the acting of a CNOT gate (solid line) and a  $\pi/4$ -one (dashed curve). The dotted-dashed curve reflects the entanglement change  $\Delta E$  between two randomly chosen pure states. b) Corresponding results for all states. The solid line corresponds to the CNOT transformation and the dashed one to the  $\pi/4$  gate.

Fig. 4-a) Mean initial entanglement  $\langle E_0 \rangle$  vs  $\Delta E$  for pure states. b) For all states. c)  $\langle E_0^2 \rangle - \langle E_0 \rangle^2$  vs.  $\Delta E$  for pure states. d) For all states. The solid line refers to the CNOT transformation and the dashed one to the  $\pi/4$  gate.

Fig. 5. Effects of the action of the CNOT gate (left) and of the  $\pi/4$ -gate (right). We plot  $P(E_F)$  vs.  $E_F$  for fixed initial entanglement  $E_0 = 0.1, 0.2, 0.3$ , and  $0.4$ , respectively.

Fig. 6 a) Mean initial entanglement  $\langle E_0 \rangle$  vs  $\Delta E$  via the CNOT gate for states with a given value of the participation rate  $R = 1.4$  and  $R = 2.2$ . b) Its associated fluctuation  $\langle E_0^2 \rangle - \langle E_0 \rangle^2$  vs.  $\Delta E$ .

fig. 1

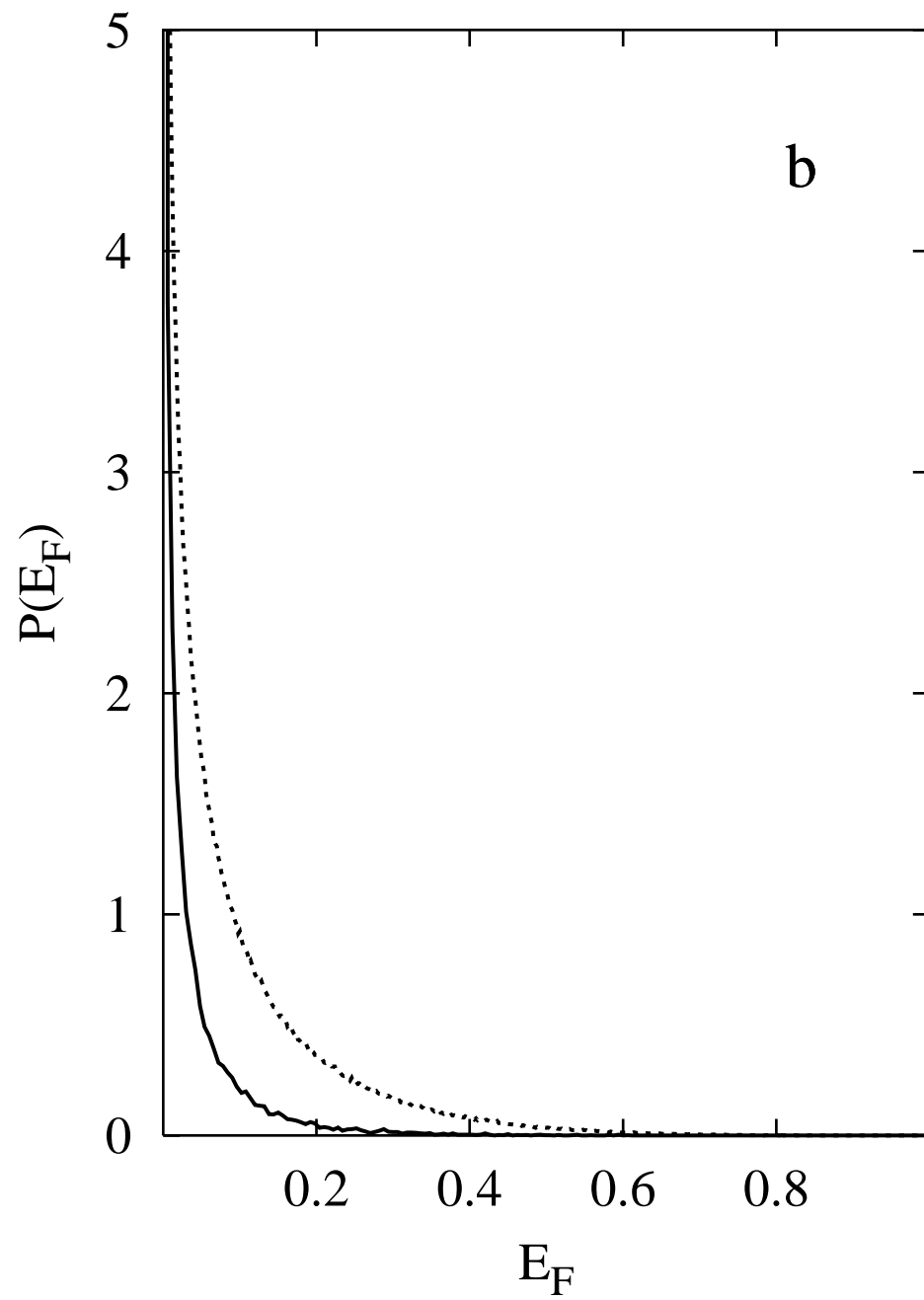
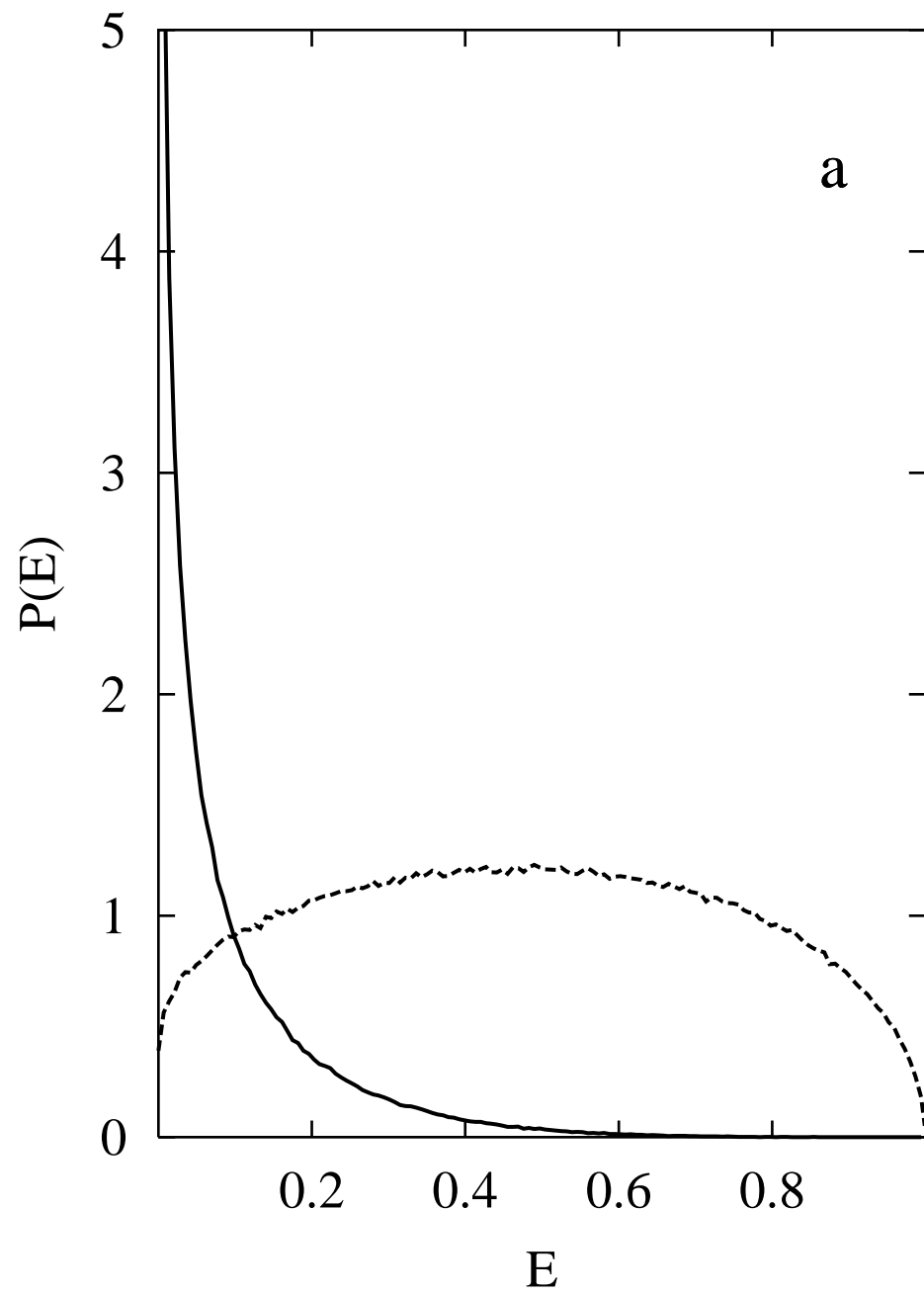




fig.2

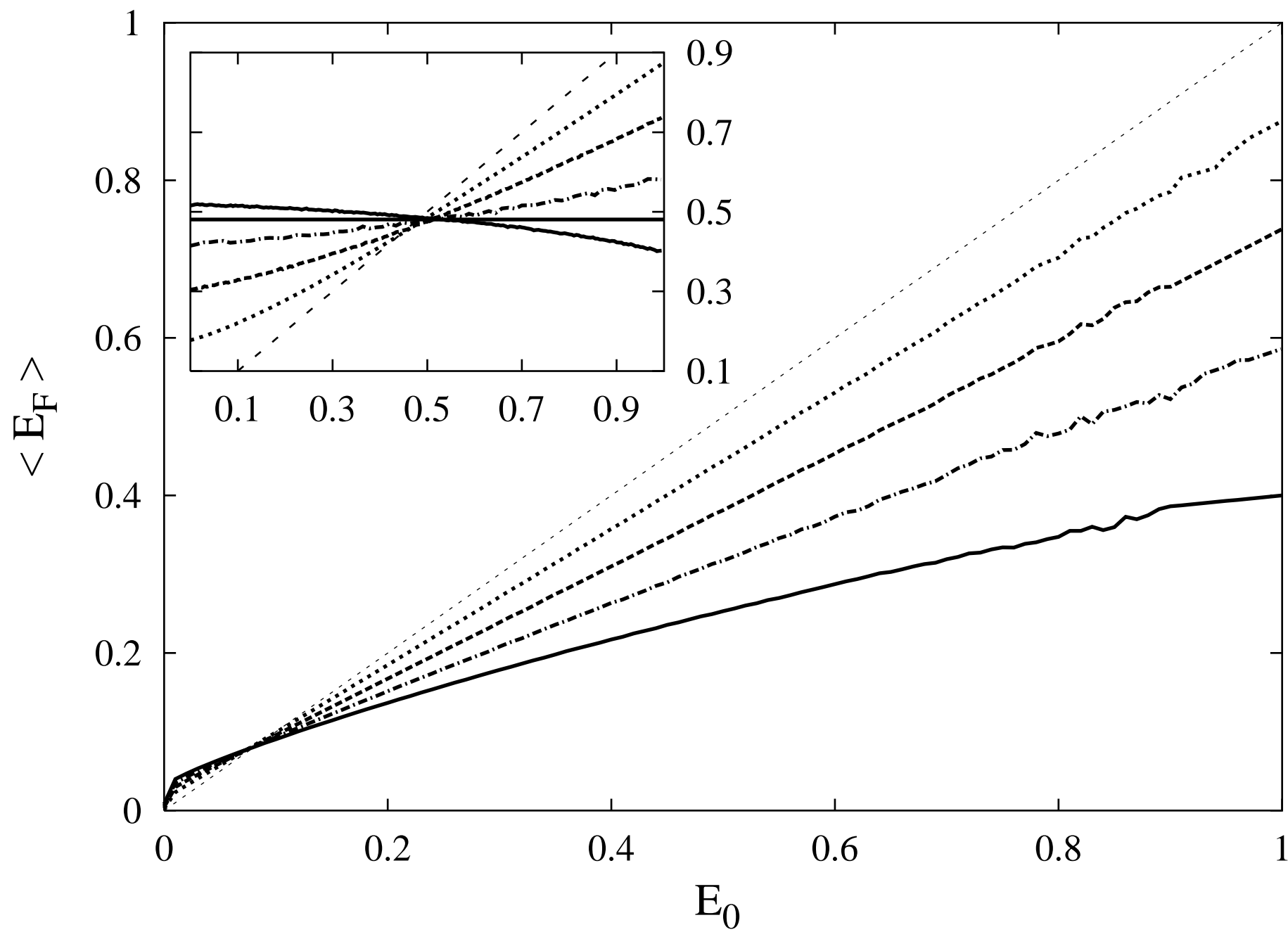


fig. 3

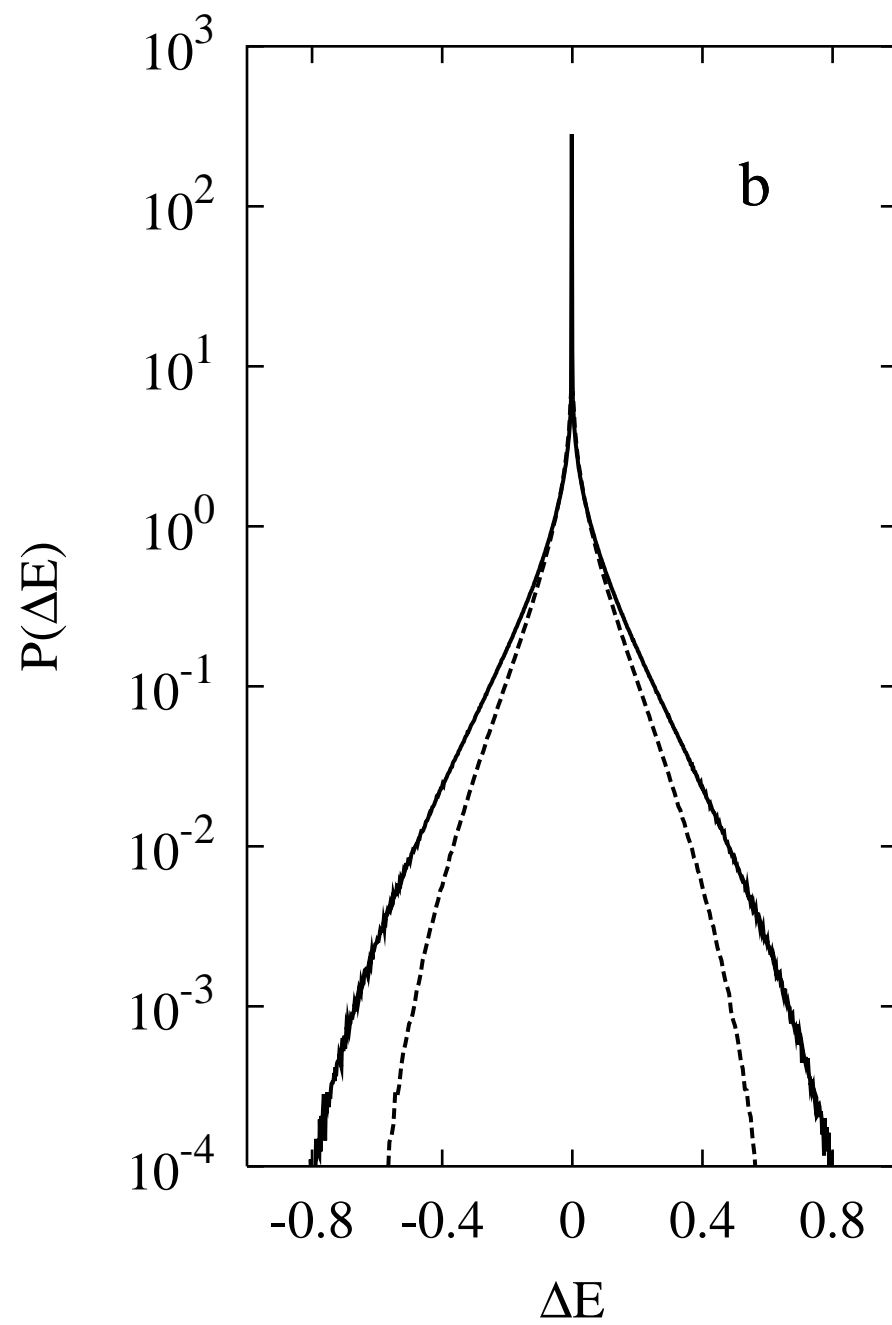
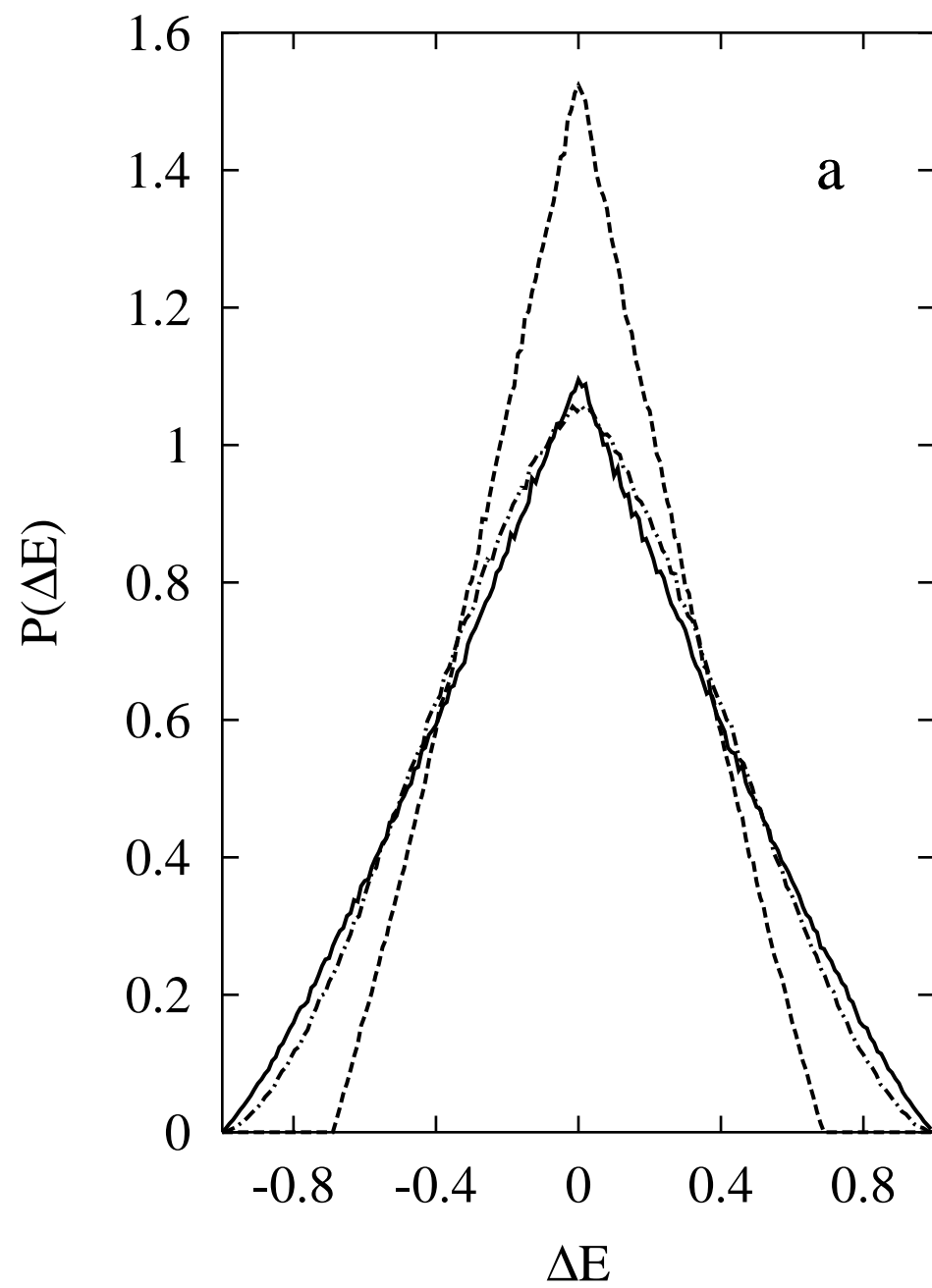


fig. 4

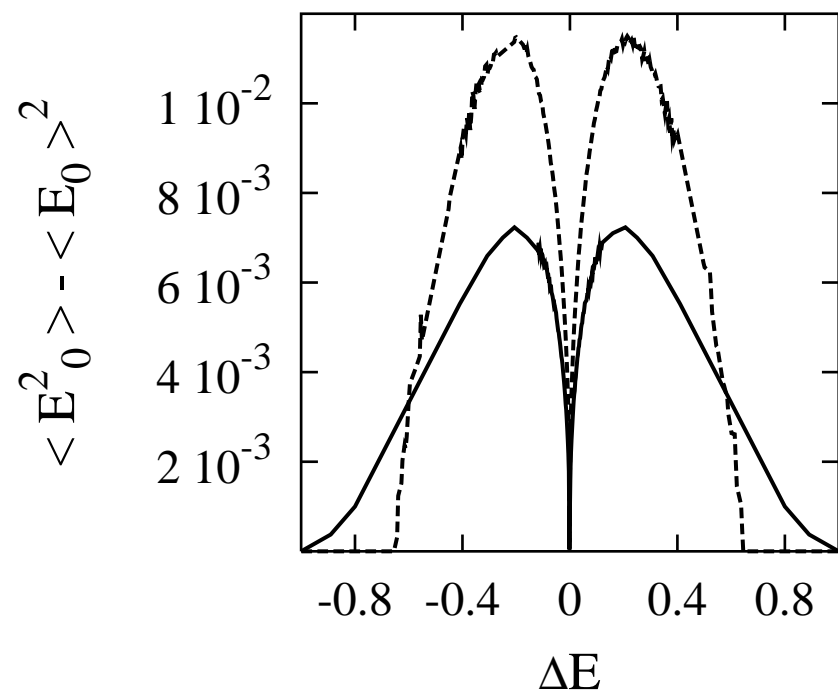
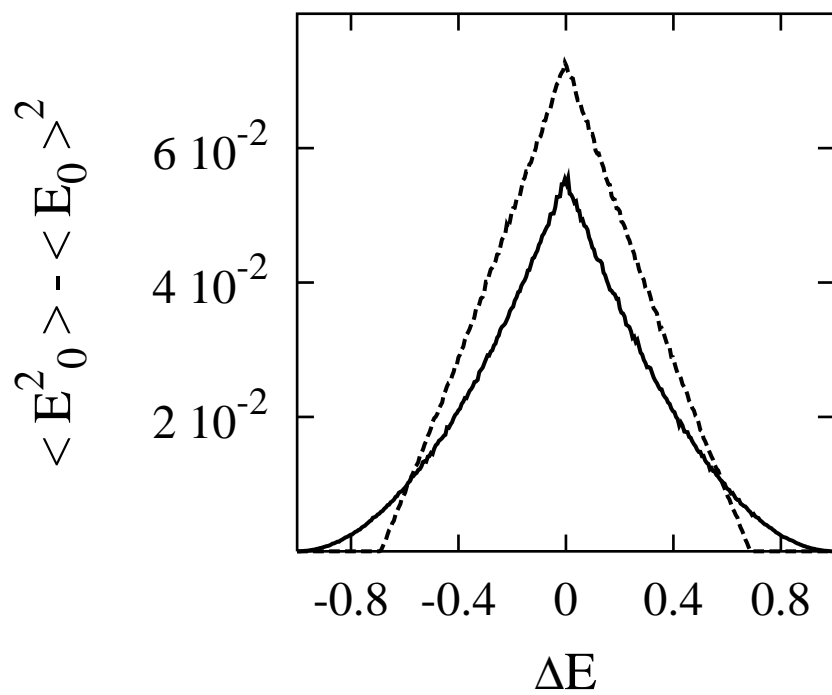
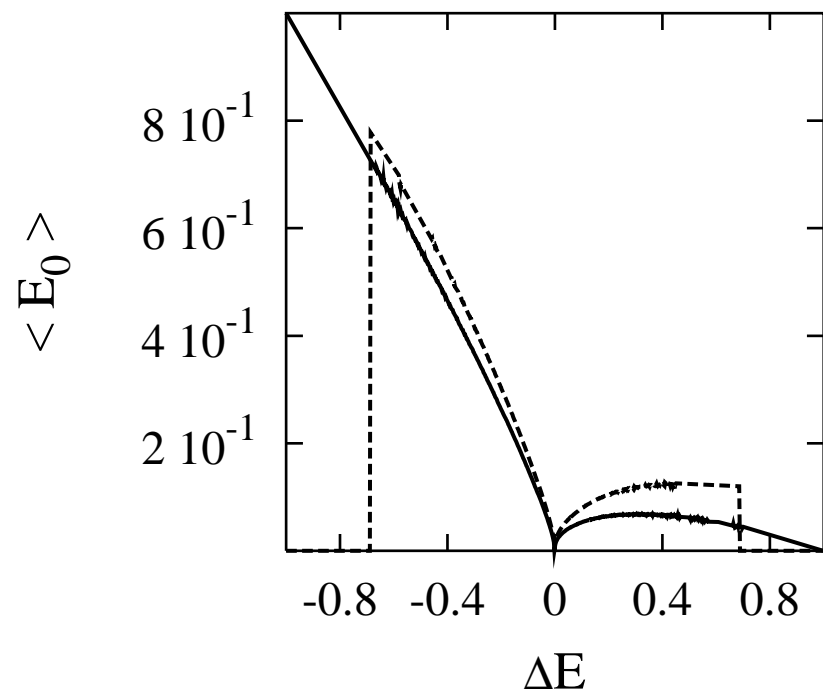
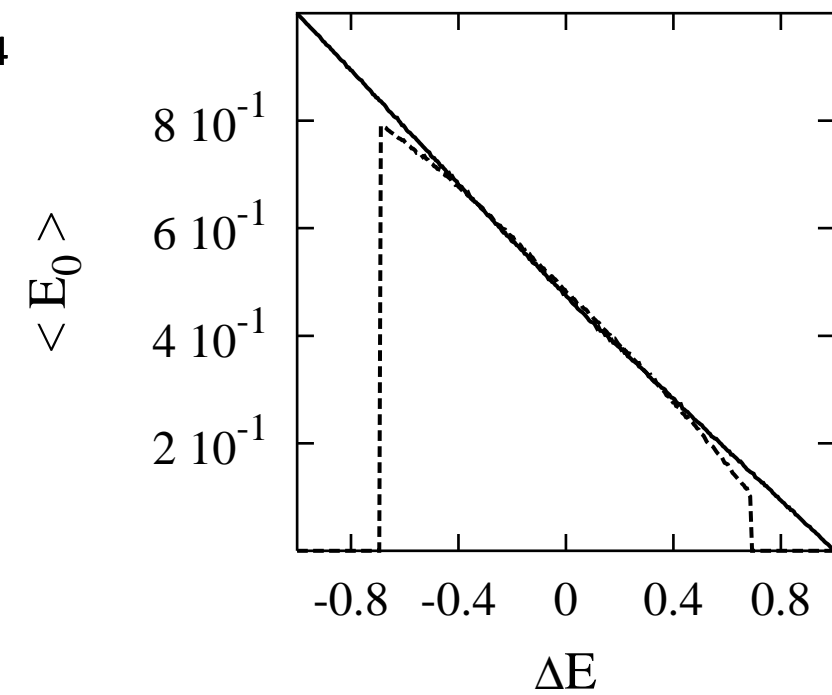


fig. 5

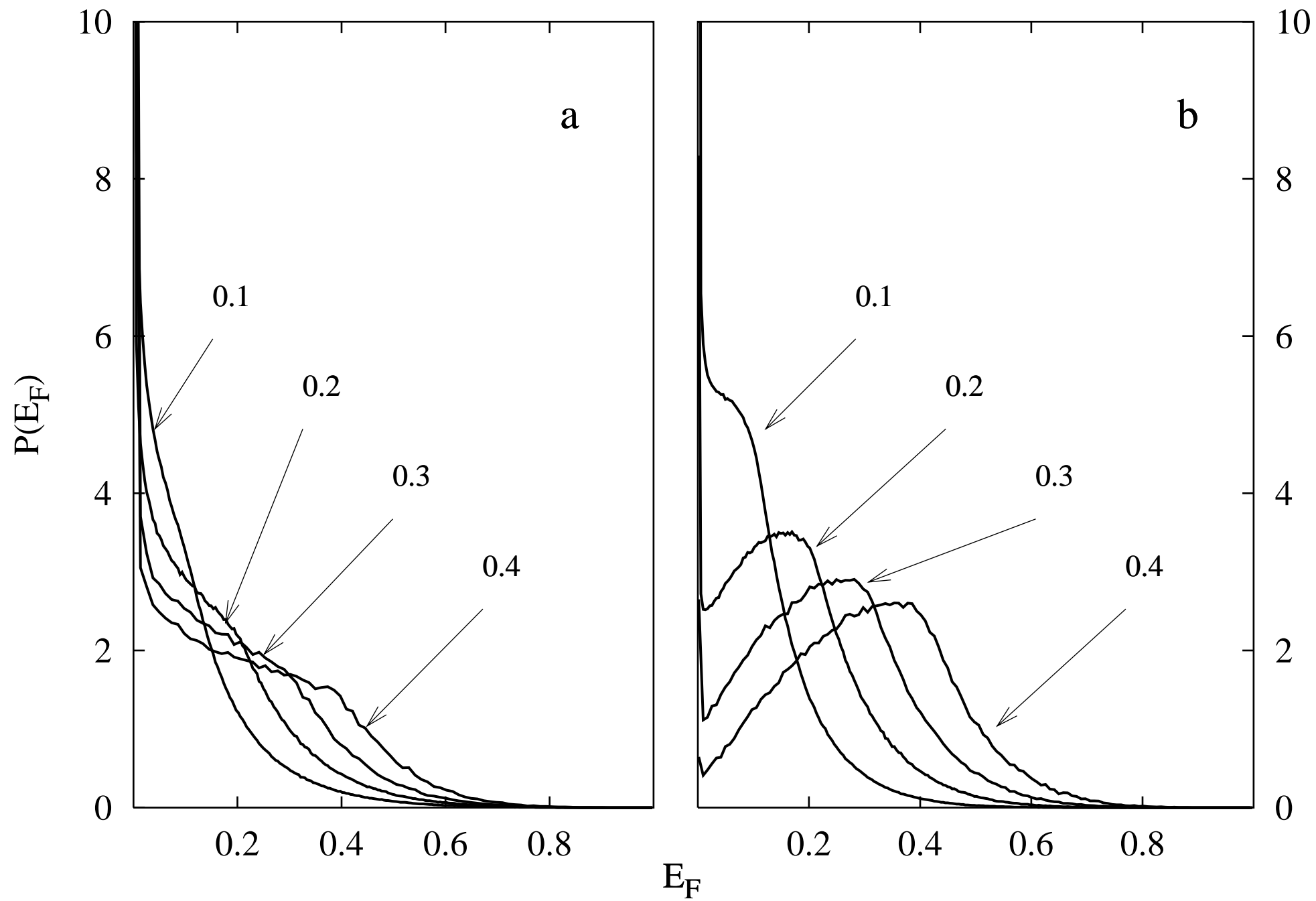


fig. 6

